May, 2019

CURRICULUM VITAE

Name:	**Gosálvez Ayuso, Miguel Angel**
Date and place of birth:	March 10, 1973; Madrid, Spain
Nationality:	Spain (NIF: 07486460Y, Passport: PAC577785)
Highest degree:	Doctor of Science in Technology - D.Sc. (Tech.), Helsinki University of Technology, 2003
Topic of highest degree:	Computational Physics
Current position:	Tenured Researcher, Dept. of Materials Physics, University of the Basque Country UPV/EHU and Donostia International Physics Center (DIPC)
Current address:	Paseo Manuel de Lardizábal 4, Donostia - San Sebastián, 20018 Gipuzkoa, Spain
Tel. / E-mail:	+34 943 015389 / miguelangel.gosalvez@ehu.es
Languages:	Spanish (native); English (fluent); Finnish (fluent); Japanese (beginner)

Research interests:

•Computational physics, multiscale modelling, surface processing
•Modeling of Micro/Nano-Electro-Mechanical Systems (MEMS and NEMS)
Etching (anisotropic, isotropic, plasma, deep reactive ion etching, focused ion beam etching,...), deposition (epitaxial/CVD growth,...), patterning,...
•Simulation methods for time evolution / front propagation / interface propagation
Kinetic Monte Carlo (KMC), Continuous Cellular Automaton (CCA), Level Set (LS), Volume of Fluid (VoF),...
•Parameter determination/optimization/calibration (e.g. atomistic rates)
First-principles (ab-initio) determination using Density Functional Theory (DFT), use of Evolutionary Algorithms (EA), Particle Swarm Optimization (PSO), Differential Evolution (DE), Evolutionary Strategies (ES), CMA-ES,...
•(Sub)monolayer growth
Epitaxial/CVD/on-surface growth, computational aspects (acceleration, paralelization,...), realistic production of 2D materials (graphene, MoS2,...)
•Relation between atomistic kinetics and macroscopic behavior
Diffusivity, activation energy (in etching, growth and heterogeneous catalysis), collective behavior (concerted motion,...)
•Graphene and other 2D materials
CVD growth, electronic/thermal transport, transistor devices,...
• Surface visualization and reconstruction (Delaunay triangulations and Level Sets)

Contents:

A. Positions and studies:

1. Tenured Researcher	University of the Basque Country (UPV-EHU), DIPC and CFM-MPC	Feb 2017 - present
2. Ramón y Cajal Researcher	University of the Basque Country (UPV-EHU), DIPC and CFM-MPC	Jun. 2010 - Jan 2017
3. GCOE Research Scientist	Dept. of Micro-Nanosystem Eng., Nagoya University, Japan	Jan. 2009 - May 2010
4. Collaborating Researcher	Helsinki Univ. of Tech., Finland	Mar. 2008 - Dec. 2008
5. Postdoctoral Researcher	Laboratory of Physics, Helsinki Univ. of Tech., Finland	Apr. 2007 - Dec. 2007
6. Assistant Professor	Sato Laboratory, Dept. of Micro-Nanosystem Eng., Nagoya University, Japan	Apr. 2006 - Mar. 2007
7. COE Research Scientist		Mar. 2004 - Mar. 2006
8. Doctor of Science in Technology	Laboratory of Physics, Helsinki Univ. of Tech., Finland	May 1998 - Sep. 2003
9. Ph.D. student (grade: 4.5 / 5)	Helsinki Univ. of Tech., Finland	May 1998 - Sep. 2003
	University of Helsinki, Finland	Jun. 1997 - Apr. 1998
10. Bilateral exchange student	X-ray Laboratory, Dept. of Physics, University of Helsinki, Finland	Sep. 1996 - May 1997
11. Licentiate in Materials Physics (grade: 7.45 / 10)	Universidad Complutense de Madrid, Spain	Sep.1991 - Sep.1996
12. ERASMUS exchange student (Diploma: 71 / 100)	University of Kent at Canterbury, UK (Last year studies in Physics with Material Physics)	Oct. 1994 - Jun. 1995

B. Participation in academic research projects:

Participation as 'principal investigator' (PI):

1. Project Title: 'Efficient simulation of deposition, patterning and etching for advanced MEMS design'
Reference: Jiangsu Province Talent Human Resource Office (2012) NO.39, project number GDJ 20143201001
Funding source: The state administration of foreign experts affairs
Received funding: 1 million CNY (approx. 147,225.21 €) [1€=6.79 CNY, 2015-03-23]
Period: Apr. 2013 - Dec. 2015
Principal Investigator: **M. A. Gosálvez**
Short description: Funding for three-year project to develop new modeling software.
Results: Commercial software: IntelliFab, FabSim and IntelliEtch, for the simulation of the various etching processes, i.e. isotropic and anisotropic wet etching, RIE and DRIE. Academic: publications in top-class MEMS journals.

2. Project Title: "Cinética macroscópica y microscópica en procesos de superficie: catálisis heterogenea, crecimiento epitaxial y ataque químico anisotrópico"
Reference: RYC-2009-05506
Funding source: Ministerio de Economía y Competitividad
Received funding: 15,000 € (additional funding for research activities)
Period: Jun. 2010 - May 2011
Principal Investigator: **M. A. Gosálvez**

3. Project Title: 'Combination of experimental and computational studies for the calibration and performance of accurate and fast simulations of anisotropic etching of silicon for MEMS applications using a Continuous Cellular Automaton (CCA)'
Reference: ---
Funding source: Wakate JSPS Young Scientist Fund, Japan Society for the Promotion of Science (JSPS), WAKATE by G-COE Dept. Micro-Nanosystems Eng., Nagoya University.
Received funding: JPY 1,000,000 (~ 7,644.58 e) [1 € = 130.81 JPY, 2015-03-23]
Period: Jun. 2009 - Mar. 2010
Principal Investigator: **M. A. Gosálvez**
Short description: Funding for collaborative visits and equipment/expriments to perform joint research with (i) the Digital Systems Design Group lead by Prof. Angel Sebastià Cortés at Universidad Politécnica de Valencia, Spain and (i) the group of Assistant Prof. Yan Xing, at the Mechanical Engineering Dept, Southeast University, Nanjing, China.
Results: Several publications (some in top-class MEMS journals), technology transfer of simulation software to a company for wet etching simulations and one PhD thesis (N. Ferrando, Universidad Politécnica de Valencia).

4. Project title: Joint Research Project 'Physical Chemistry of Anisotropic Chemical Etching of Silicon Applied for MEMS' (Bilateral program between JSPS, Japan and AKA, Finland)
Funding source: Japan Society for the Promotion of Science (JSPS)
Received funding: JPY 9,500,000 (72,630.09 €, 1€=130.81 JPY, 2015-03-23)
Period: Oct. 2005 - Sept. 2007 (funding for frequent visits and organization of workshops)
Principal Investigators: K. Sato and **M. A. Gosálvez**
Results: Numerous publications in physical, computational and microengineering journals (some

in top-class MEMS journals) and one PhD thesis (D. Cheng, Nagoya University).
Short description of B.4 and B.6: Funding for collaborative visits and organization of international workshops (www.fyslab.hut.fi/~tjh/workshop.html and www.fyslab.hut.fi/~tjh/workshop07.html). The collaboration was extended to incorporate the Dept. of Physics, Nagoya University (Prof. M. Uwaha) and Denso Corp., Japan (Dr. H. Tanaka).
Results: More than a dozen publications (some in top-class MEMS journals) and one PhD thesis (T. Hynninen, Helsinki University of Technology, now Aalto University).

Participation as group member:

5. Project title: The design and analysis tools for the coupling of multi-physics in MEMS
Reference: BK2008311
Received funding: 250,000 CNY (Chinese Yuan, ~35,000 €, 1€=6.79 CNY, 2015-03-23)
Funding source: Southeast University, Nanjing, China and Jiangsu IntelliSense Technology Co., Ltd., China
Period: Jan. 1, 2009 - Dec. 31, 2009
Principal Investigator: Yan Xing, Dept. of Mechanical Engineering, Liu Longhu Campus, Southeast University, Jianging Section, Nanjing 211189, China
Short description: Funding for collaborative visits to perform joint research between Southeast University, IntelliSense Co. and Nagoya University, Japan.
Results: Several publications and technology transfer of simulation software to a company for wet etching simulations.

6. Project Title: Joint Research Project 'Role of metal impurities and etchant cations during anisotropic etching' (Bilateral program between JSPS, Japan and AKA, Finland)
Reference: SA 122603
Funding source: The Finnish Academy of Science and Letters (AKA)
Received funding: 150,000 € (funding for frequent visits and organization of workshops)
Period: Sep. 2005 - Dec. 2007
Principal Investigators: R. Nieminen and A. Foster (AKA)
(see B.4 above)

7. Project title: JSPS Scientific Research (A): Research on wet anisotropic etching model of single crystal silicon and effects of cation components in the solution
Reference: 19201026
Funding source: Japan Society for the Promotion of Science (JSPS)
Received funding: JPY 34,000,000
Period: Apr. 1, 2007 - Mar. 31, 2010
Principal Investigator: K. Sato

8. Project title: Japanese MEXT 21st Center of Excellence Program "Micro' and Nano - Mechatronics for Information' Base d Society" (2003-2007)
Reference: H-010
Funding source: Japan Society for the Promotion of Science (JSPS)
Received funding: JPY 831,280,000 (6,367,367.88 €, 1€=130.81 JPY, 2015-03-23)
Period: Jul. 2003 - Mar. 2008
Principal Investigators: Y. Mitsuya (leader) and 6 sub-leaders including K. Sato

9. Project title: Global Center of Excellence Program of Japan, Dept. of Micro'Nanosystems Engineering, Nagoya University
Reference: H-017

Funding source: Japan Society for the Promotion of Science (JSPS)
Received funding: JPY l,390,868,000 (10,644,641.04 €, 1€=130.81 JPY, 2015-03-23)
Period: Jul. 2008 - Mar. 2013
Principal Investigators: T. Fukuda (leader) and 17 members including K. Sato

10. Project Title: Center of Excellence in Computational Nanoscience (COMP)
Reference: 2006-2011
Funding source: The Finnish Academy of Science and Letters (AKA)
Period: 2006 - 2011
Principal Investigator: R. M. Nieminen
Results: Several publications.

11. Project Title: Center of Excellence in Computational Nanoscience (COMP)
Reference: 2000-2005
Funding source: The Finnish Academy of Science and Letters (AKA)
Period: 2000 - 2005
Principal Investigator: R. M. Nieminen
Results: Several publications.

12. Project Title: 'Piezoelectric and ferroelectric properties of perovskites'
Reference: ---
Funding source: The Finnish Academy of Science and Letters (AKA)
Period: 2005 - 2008
Principal Investigator: R. M. Nieminen
Results: Several publications.

13. Project Title: 'Reactive flows'
Reference: ---
Funding source: The Finnish Academy of Science and Letters (AKA)
Period: 1998 - 2003
Principal Investigator: R. M. Nieminen
Results: Six publications and one PhD thesis (M. A. Gosalvez, Helsinki University of Technology, now Aalto University).

(Rejected) European/National projects, participation as 'principal investigator' (PI):

14. Project Title: European coordinated funding proposal 'CVDgrapheneLAB — Tailored graphene production from growth kinetics to device fabrication'
Call: 'ICT-2011.9.1 FET-Open, Challenging current thinking', September 2012

15. Project Title: European coordinated funding proposal 'Evolutionary Kinetics for Transport - Multiscale evolutionary modeling of surface-mediated growth, transport properties and electronic devices'
Call: 'FP7-NMP-2013-SMALL-7', October 2012

16. Project Title: National coordinated funding proposal 'Numerical engineering of low-dimensional materials and nanostructures (NEMN)'
Call: Programa Estatal de I+D+i Orientada a los Retos de la Sociedad, Ministerio de Economía y Competitividad (MINECO), April 2016

C. Technology transfer / participation in research contracts with companies:

1. Morfokinetics
Funding source: Grupo SPRI and Diputación de Guipúzcoa
Received funding: 30,000 €
Period: Nov. 2013 - Nov. 2014
Purpose: Prototype development for start-up company.

2. Development of simulation tools for MEMS and NEMS applications
Funding source: IntelliSense Software Corp., Boston, Massachusetts, USA
Received funding: USD 29,218.70 (approx. 22,597.60 e) [1e=1.293 USD, 2012-09-28]
Period: Sep. 2011 - Mar. 2012
Purpose: Tool development (SprayEtch) and customer support. Worldwide commercialization (http://www.intellisensesoftware.com/).

3. Software licensing agreement
Funding source: IntelliSense Software Corp., Boston, Massachusetts, USA
Received funding: approx. 35,000.00 e
Period: Feb. 2008 -
Purpose: Tool development (VisualTAPAS, now IntelliEtch) and customer support. Worldwide commercialization (http://www.intellisensesoftware.com/).

4. Advice on implementation, calibration and use of atomistic algorithms for simulating anisotropic etching of crystalline silicon and similar materials
Funding source: Coventor, Inc., 4000 Centre Green Way, Suite 190, Cary, NC27513, USA
Received funding: approx. 2,000.00 e
Period: Jan. 2005 - Dec. 31, 2006
Purpose: Software testing and evaluation, tool development and customer support.

CAD software provided by both companies (IntelliSense and Coventor) is used by engineers at major semiconductor and electronics companies worldwide to develop leading edge micro- and nano-scale sensors and devices.

D. Academic grants, awards, prizes, honors and distinctions:

1. Mar 2015, UNIBASQ certificate for employment as 'Personal doctor investigador'.
2. Mar 2015, UNIBASQ certificate for employment as 'Profesor adjunto'.
3. Aug 2014, 'I3 Program Certificate' from MINECO for "satisfying the requirements of quality in scientific/technological activity and production" within the Ramón y Cajal Program by Ministerio de Ciencia e Innovación, now M. Economía y Competitividad. I3 = Incentivación de la Incorporación e Intensificación de la Actividad Investigadora.
4. Feb 2012, [Gosálvez *et al.*, J. Micromech. Microeng. 21 (2011) 065017] is featured in JMM's 'Highlights Collection of 2011'. (http://iopscience.iop.org/0960-1317/page/

Highlights%20of%202011)

5. Jan 2012, [Ferrando *et al.*, GPUetch: A Fast and Accurate Wet Etching Simulator for Silicon and Quartz MEMS] wins the Modeling and Simulation of Nano/Microsystems Contest, organized by the National Nanotechnology Infrastructure Network (NNIN) and the University of Michigan, "NNIN/C at Michigan Fall Contest", autumn 2011.
6. May 2011, [Gosálvez *et al.*, J. Micromech. Microeng. 21 (2011) 065017] is chosen as 'IOP Select' article. (Novelty, significance and potential impact on future research, www.iop.org/Select/)
7. Nov 2009, JMEMS lapel pin award for 'his diligence and care in reviewing, and his efforts in support of JMEMS and our research field.'
8. Mar 2009, [Gosálvez *et al.*, J. Micromech. Microeng. 18 (2008) 055029] is featured in JMM's 'Highlights Collection of 2008'. (http://iopscience.iop.org/0960-1317/page/Highlights%20of%202008)
9. May 2008, [Gosálvez *et al.*, J. Micromech. Microeng. 18 (2008) 055029] is chosen as 'IOP Select' article. Novelty, significance and potential impact on future research, www.iop.org/Select/)
10. Dec 2004, 8,000 € grant award for designated activities from the Finnish Academy of Science and Letters, Vilho, Yrjö and Kalle Väisälä Foundation.
11. Nov 2004, [Gosálvez and Sato, Exploring the activation energy during nanoscale structural evolution in wet etching] wins the Best Paper Award in The 2004 International Symposium on Micro-NanoMechatronics and Human Science (MHS2004), Nagoya, Japan.
12. Dec 2003, 10,000 € grant award for travel and settling expenses from the Finnish Academy of Science and Letters, Vilho, Yrjö and Kalle Väisälä Foundation.
13. Year 2002, Gosálvez's research is highlighted in "MathInsight 2002" international calendar, Editors Hans-Christian Hege, Konrad Polthier and Martin Rumpf, Springer-Verlag, Germany.
14. Dec 2, 2001, Gosálvez's research is highlighted in the "FAZ am Sonntag" sunday edition of the daily "Frankfurter Allgemeine Zeitung", Frankfurt, Germany.

E. Invited talks:

1. M. A. Gosálvez, J. Alberdi-Rodriguez, 'Another approach to heterogeneous catalysis', ACS Spring 2019 National Meeting, Session in 'Advances in Methods for Comparing Molecular & Supramolecular Simulations to Experiments', Division of 'Catalysis Science and Technology', Orange County Convention Center, Orlando, Florida, USA, March, 31, 2019.
2. 'Recent developments in the IntelliEtch module - Anisotropic etching, corner compensation, isotropic etching, etc', IntelliSense Workshop, Jiangsu IntelliSense Technology Co., Ltd., Nanjing, China, August 20, 2013.
3. 'Reliable atomistic simulations of anisotropic etching for MEMS applications, MEMS for personal life, Nagoya University, Nagoya, Japan, March 1-2, 2012.
4. 'New features in IntelliEtch', IntelliSense Workshop, Jiangsu IntelliSense Technology Co., Ltd., Nanjing, China, June 11-12, 2011.
5. 'Recent advancements in the simulation of anisotropic etching for microengineering

applications', Department of Mechanical Engineering, Southeast University, Nanjing, China, June 10, 2011.
6. 'VisualTAPAS: an example of DFT-assisted understanding and simulation of anisotropic etching', Theory Meets Industry, Erwin-Schrdinger-Institute for Mathematical Physics, Wien, Austria, June 12-14, 2007. [*J. Phys.-Condens. Matter* **20** (2008) 064234].
7. 'Atomististic simulation of anisotropic etching', Towards Reality in Nanoscale Materials', Levi, Finland, December 10-12, 2007.
8. 'An atomistic introduction to anisotropic etching', Fifth International Workshop on Physical Chemistry of Wet Etching of Semiconductors, PCWES 2006, Saarbrücken, Germany, June 19 - 21, 2006.

F. Publication metrics and outstanding articles:

Date: 2018.01.29	***Web of Science (WS)***	***Research Gate (RG)***	***Google Scholar (GS)***
***Articles** (WCD)*	***73** (65)*	***79** (69)*	***84** (68)*
Citations	*807*	*1017*	*1320*
Citations per Item	*12,42*	*14,74*	*19,41*
h-index	***17***	***18***	***22***
Other info	*ID: H-1054-2012*	*RG Score: 31.95*	*i10-index: 35*

WCD = With Citation Data

Citation data shown below regarding WS, RG and GS correspond to 2018.01.29

F.1 Highest impact factor:

K. M. McPeak, C. D. van Engers, M. Blome, J. H. Park, S. Burger, M. A. Gosálvez, A. Faridi, Y.R. Ries, A. Sahu and D. J. Norris, Complex Chiral Colloids and Surfaces via High-Index Off-Cut Silicon, *Nano Letters*, 2014, 14 (5), pp 2934–2940.
DOI: 10.1021/nl501032j
2014 IF 13.592 (2014 8/157 Q1 T1 in Multidisciplinary Chemistry)
Citations = 22 WS, 23 RG, 28 GS.
Manufacture of chiral surface structures and particles with specific handedness using plasmonic metals. Record molar circular dichroism at red wavelengths and chiral optical signatures resonant with biomolecules in the ultraviolet.

F.2 Most cited:

M. A. Gosálvez, K. Sato, A. S. Foster, R. M. Nieminen, and H. Tanaka, An atomistic introduction to anisotropic etching, *J. Micromech. Microeng.* **17** (2007) S1-S26.
DOI: 10.1088/0960-1317/17/4/S01
2007 IF 1.930 (1st class MEMS journal; 2007 29/227 Q1 T1 in Electrical & Electronic Engineering). Citations = 67 WS, 74 RG, 101 GS.
Review article.

F.3 Fundamental for 'IntelliEtch' commercial simulator:

N. Ferrando, M. A. Gosálvez, J. Cerdà, R. Gadea, and K. Sato, Octree-based, GPU Implementation of a Continuous Cellular Automaton for the Simulation of Complex,

Evolving Surfaces, *Comput. Phys. Commun.* **182** (2011) 628-640.
DOI: 10.1016/j.cpc.2010.11.004
2011 IF 3.268 (2011 10/99 Q1 T1 in Interdisciplinary Applications of Computer Science). Citations = 21 WS, 27 RG, 34 GS.
The performance of desktop parallel computing using Graphics Processing Units (GPUs) has dramatically increased in the last years. Accordingly, the paper presents a GPU implementation of a continuous cellular automaton, efficiently utilizing the large amount of processors available in typical graphics cards. This has a direct impact on the overall simulation efficiency, achieving two-orders-of-magnitude faster executions over traditional computing architectures based on single Central Processing Units (CPUs).

F.4 Fundamental for 'Morfokinetics' start-up initiative:
N. Ferrando, M. A. Gosalvez, and A. Ayuela, Evolutionary Kinetic Monte Carlo - Atomistic Rates of Surface-Mediated Processes from Surface Morphologies, J. Phys. Chem. C, 2014, 118 (22), pp 11636–11648.
DOI: 10.1021/jp409812x
2014 IF 4.772 (2014 29/139 Q1 T1 in Physical Chemistry).
Citations = 3 WS, 2 RG, 7 GS.
Theory and simulation at the nanoscale. Extracting reactivity from morphology.

F.5 First combination of Evolutionary Algorithms and Kinetic Monte Carlo:
Y. Xing, M. A. Gosálvez, K. Sato, M. Tian and H. Yi, Evolutionary determination of Kinetic Monte Carlo rates for the simulation of evolving surfaces in anisotropic etching of silicon, *J. Micromech. Microeng.* **22** (2012) 085020 (12pp).
DOI: 10.1088/0960-1317/22/8/085020
2012 IF 1.790 (1st class MEMS journal; 2012 65/243 Q2 T1 in Electrical & Electronic Engineering; 2012 56/827 Q1 T1 in Engineering). Citations = 6 WS, 7 RG, 12 GS.
We use an evolutionary algorithm (EA) to determine the atomistic rates for the simulation of anisotropic etching of silicon using the Kinetic Monte Carlo (KMC) method for the manufacture of microelectromechanical systems (MEMS). This method has been extended to other surface-mediated processes (see item 4 above).

F.6 Featured in 'Highlights Collection of 2011' by 'IOPselect':
M. A. Gosálvez, N. Ferrando, Y. Xing, Prem Pal, K. Sato, J. Cerdà, R. Gadea, Simulating anisotropic etching of silicon in any etchant: Evolutionary algorithm for the calibration of the continuous cellular automaton, *J. Micromech. Microeng.* **21** (2011) 065017 (15pp).
DOI: 10.1088/0960-1317/21/6/065017
2011 IF 2.105 (1st class MEMS journal; 2011 47/245 Q1 T1 in Electrical & Electronic Engineering). Citations = 13 WS, 14 RG, 17 GS.
IOPselect status based on novelty, significance and potential impact on future research. We use an evolutionary algorithm (EA) to determine the atomistic rates for the simulation of anisotropic etching of silicon in many widely different and technologically relevant etchants using the Continuous Cellular Automaton (CCA). The proposed calibration model is the basis for a commercial simulator known as IntelliEtch (Section C.3).

F.7 Featured in 'Highlights Collection of 2008' by 'IOPselect':

M. A. Gosálvez, Y. Xing, K. Sato, and R. M. Nieminen, Atomistic methods for the simulation of evolving surfaces, *J. Micromech. Microeng.* **18** (2008) 055029 (17pp).
DOI: 10.1088/0960-1317/18/5/055029

2008 IF 2.233 (1st class MEMS journal; 2008 44/229 Q1 T1 in Electrical & Electronic Engineering). Citations = 22 WS, 23 RG, 37 GS.

A detailed review on the pros and cons of various Kinetic Monte Carlo (KMC) and Cellular Automata (CA) methods used for simulating the time propagation of an advancing surface. The paper also describes the optimal procedure to define an underlying substrate structure using an octal tree in order to perform the simulations using a minimal amount of memory. It also describes several physical models to assign values to the process rates required as the input for the KMC and CA simulations. IOPselect status based on novelty, significance and potential impact on future research.

F.8 Combining Firstprinciples DFT and Kinetic Monte Carlo:

T. Hynninen, A. S. Foster, M. A. Gosálvez, R. M. Nieminen, and K. Sato, Adsorption of metal impurities on H-terminated Si surfaces and their effect on wet etching of Si, *J. Phys.-Condens. Matter* **20** (2008) 485005 (9pp).
DOI: 10.1088/0953-8984/20/48/485005

2008 IF 1.900 (2008 17/62 Q2 T1 in Condensed Matter Physics)
Citations = 3 WS, 5 RG, 4 GS.

A good example of the so called First-principles Kinetic Monte Carlo (FP-KMC) approach which combines DFT calculations for the determination of adsorption/desorption energetics and KMC simulations to determine the overall time evolution (kinetics). We used DFT calculations in order to characterize the adsorption energies and clustering properties of some metals such as Cu, Pb and Mg on the H/OH-terminated silicon surface during etching, and KMC simulations to describe the effect of these impurities on the surface morphology and etch rates of {100} and {110}, obtaining a good qualitative agreement with the experiments. A similar approach has been used by different research groups around the world in order to accurately understand industrially relevant processes, such as the heterogeneous catalysis of the oxidation of CO [Reuter and Scheffler, *Phys. Rev. B* **73** (2006) 045433] or the production of ammonia [Honkala et al., *Science* **307** (2005) 555].

F.9 Most satisfying:

M. A. Gosálvez, D. Cheng, R. M. Nieminen and K. Sato, Apparent activation energy during surface evolution by step formation and flow, *New J. Phys.* **8** (2006) 269 (11pp).
DOI: 10.1088/1367-2630/8/11/269

2006 IF 3.754 (2006 9/68 Q1 T1 in Multidisciplinary Physics)
Citations = 12 WS, 14 RG, 14 GS.

By considering that wet etching is essentially a step flow process resulting from the removal of kink atoms at morphological steps, we explain the orientation dependence of the apparent activation energy, a traditionally debated feature in the field. Contrary to

extended believe, we showed that the activation energy can display a minimum for unreactive surfaces, such as Si{111}, as claimed by some experiments considered controversial before our report. This study indicated that the concept of a rate-limiting reaction (or "bottle-neck" process, whose activation energy is the largest between all possible processes) is not valid for anisotropic etching. We are currently applying similar ideas to describe the overall activation energy in heterogeneous catalysis and epitaxial growth.

F.10 Most challenging theoretical achievement:

M. A. Gosálvez, M. M. Otrokov, N. Ferrando, A. G. Ryabishchenkova, A. Ayuela, P. M. Echenique, and E. V. Chulkov, Low-coverage surface diffusion in complex periodic energy landscapes: Analytical solution for systems with symmetric hops and application to intercalation in topological insulators, *Phys. Rev. B* **93**, 075429 (2016).
DOI: 10.1103/PhysRevB.93.075429
2016 IF 3.836 (2016 18/67 Q2 T1 in Condensed Matter Physics)
Citations = 3 WS, 4 RG, 6 GS.
Theoretical derivation and computational validation of general diffusivity formulae and description of the latest experiments on diffusion of metals on topological insulators.

G. List of publications:

International *peer-reviewed* papers: 84.
Book chapters (4), PhD thesis (1), papers in international *peer-reviewed* journals (60), papers in *peer-reviewed* proceedings of international conferences (24), presentations in international workshops (26), presentations during collaboration visits (11, since 2009).

Book chapters: (4)

1. M. A. Gosálvez, Modeling of Silicon Etching, Ch. 12 in Part II of *Handbook of Silicon Based MEMS Materials and Technologies* (Second Edition), Eds. M. Tilli, T. Motooka, V.-M. Airaksinen, S. Franssila, M. Paulasto-Kröckel and V. Lindroos, Elsevier, Micro and Nano Technologies series. (Jan. 2015) pp. 333-353.
   DOI: 10.1016/B978-0-323-29965-7.00012-9
   Citations = 0 WS, 0 RG, 0 GS.
2. M. A. Gosálvez, I. Zubel, E. Viinikka, Wet etching of Silicon, Ch. 22 in Part IV of *Handbook of Silicon Based MEMS Materials and Technologies* (Second Edition), Eds. M. Tilli, T. Motooka, V.-M. Airaksinen, S. Franssila, M. Paulasto-Kröckel and V. Lindroos, Elsevier, Micro and Nano Technologies series. (Jan. 2015) pp. 470-502.
   DOI: 10.1016/B978-0-8155-1594-4.00024-3
   Citations = 0 WS, 4 RG, 0 GS.
3. M. A. Gosálvez, Manufacture and processing of MEMS structures, Ch. 10 in Part II of *Handbook of Silicon Based MEMS Materials and Technologies*, Chapter Editors R. M. Nieminen and T. Motooka, Book Editors V. K. Lindroos, M. Tilli, A. Lehto and T. Motooka, Elsevier, Micro and Nano Technologies series. (Jan. 2010) pp. 157-177.
   DOI: 10.1016/B978-0-8155-1594-4.00010-3
   Citations = 0 WS, 0 RG, 3 GS.

4. M. A. Gosálvez, I. Zubel, E. Viinikka, Wet etching of Silicon, Ch. 24 in Part IV of *Handbook of Silicon Based MEMS Materials and Technologies*, Chapter Editor H. Seidel, Book Editors V. K. Lindroos, M. Tilli, A. Lehto and T. Motooka, Elsevier, Micro and Nano Technologies series. 55 pages. (Jan. 2010) pp. 375-407.
   DOI: 10.1016/B978-0-8155-1594-4.00024-3
   Citations = 12 WS, 16 RG, 23 GS.

PhD thesis: (1)

Atomistic Modeling of Anisotropic Etching of Crystalline Silicon, Dissertation 123 (2003), Dissertations of Laboratory of Physics, Helsinki University of Technology, Finland. **Citations = 0 WS, 7 RG, 17 GS.**

Papers in international peer-reviewed journals: (60)

2019:

1. Z. Guo, Y. Xing, Miguel A. Gosálvez, G. Wu, X. Qiu, Characterization of anisotropic wet etching of single-crystal sapphire, Submitted.
2. J. Alberdi-Rodriguez, Shree Ram Acharya, T. S. Rahman, A. Arnau, M. A. Gosálvez, On the validity of the Arrhenius picture in two-dimensional submonolayer growth, Submitted.
3. M. A. Gosálvez and J. Alberdi-Rodriguez, An alternative perspective on heterogeneous catalysis, Submitted.

2018:

4. Y. Xing, J. Zhang, M. A. Gosálvez, H. Zhang, Y. Li, S. Zhou, The Maximum Positive Curvature Recognition Method to Determine Etch Profiles in Wet Etching of Quartz on AT and BT cuts, *J. Microelectromech. Syst.*, 2018, **27** (4), 730-738. DOI: 10.1109/JMEMS.2018.2850442
   2016 IF 2.124 (1st class MEMS journal; 2015 29/132 Q1 T1 in Mechanical Engineering ; 2016 105/262 Q2 T2 in Electrical & Electronic Engineering).
   Citations = 0 WS, 0 RG, 0 GS.

2017:

5. Y. Xing, M. A. Gosálvez, H. Zhang, and Y. Li, Transient and stable profiles during anisotropic wet etching of quartz, *J. Microelectromech. Syst.*, 2017, **26** (5), pp 1063 - 1072. DOI: 10.1109/JMEMS.2017.2707096
   2016 IF 2.124 (1st class MEMS journal; 2015 29/132 Q1 T1 in Mechanical Engineering ; 2016 105/262 Q2 T2 in Electrical & Electronic Engineering).
   Citations = 0 WS, 0 RG, 0 GS.
6. M. A. Gosálvez and J. Alberdi-Rodriguez, Microscopic Origin of the Apparent Activation Energy in Diffusion-mediated Monolayer Growth of Two-Dimensional

Materials, *J. Phys. Chem. C*, 2017, **121** (37), pp 20315–20322.
DOI: 10.1021/acs.jpcc.7b05794
2016 IF 4.536 (2016 31/146 Q1 T1 in Physical Chemistry).
Citations = 0 WS, 0 RG, 0 GS.

7. H. Zhang, Y. Xing, Y. Li, M. A. Gosálvez, X. Qiu, Kinetic Monte Carlo method for the simulation of anisotropic wet etching of quartz, *Sens. Actuator A-Phys.* **256** (2017) pp. 24–34. DOI: 10.1016/j.sna.2017.01.008
2016 IF 2.499 (1st class MEMS journal; 2016 86/262 Q2 T1 in Electrical & Electronic Engineering; 2016 52/861 Q1 T1 in Engineering).
Citations = 0 WS, 0 RG, 0 GS.

2016:

8. M. A. Gosálvez, Y. Li, N. Ferrando, P. Pal, K. Sato, Y. Xing, Fluctuations during anisotropic etching: Local recalibration and application to Si{110}, *J. Microelectromech. Syst.* **25** (2016) 788-798. DOI: 10.1109/JMEMS.2016.2562026
2016 IF 2.124 (1st class MEMS journal; 2015 29/132 Q1 T1 in Mechanical Engineering; 2016 105/262 Q2 T2 in Electrical & Electronic Engineering).
Citations = 1 WS, 3 RG, 3 GS.
Experimental and physical modeling.
9. M. A. Gosálvez, N. Ferrando, Y. Fedorshyn, J. Leuthold, J. K. McPeak, Evidence for faster etching at the mask-substrate interface: atomistic simulation of complex cavities at the micron-/submicron- scale by the continuous cellular automaton, *J. Micromech. Microeng.* **26** (2016) 045013 (10pp). DOI: 10.1088/0960-1317/26/4/045013
2016 IF 1.794 (1st class MEMS journal; 2016 121/262 Q2 T2 in Electrical & Electronic Engineering; 2016 84/861 Q1 T1 in Engineering).
Citations = 1 WS, 2 RG, 1 GS.
Experiment and simulation of anisotropic etching at the nanoscale.
10. M. A. Gosálvez, M. M. Otrokov, N. Ferrando, A. G. Ryabishchenkova, A. Ayuela, P. M. Echenique, and E. V. Chulkov, Low-coverage surface diffusion in complex periodic energy landscapes. II. Analytical solution for systems with asymmetric hops, *Phys. Rev. B* **93** 205416 (2016). DOI: 10.1103/PhysRevB.93.205416
2016 IF 3.836 (2016 18/67 Q2 T1 in Condensed Matter Physics).
Citations = 1 WS, 1 RG, 2 GS.
New, real-space, exact analytical procedure to determine the tracer diffusivity in periodic systems, as an alternative to the traditional reciprocal space approach.
11. M. A. Gosálvez, M. M. Otrokov, N. Ferrando, A. G. Ryabishchenkova, A. Ayuela, P. M. Echenique, and E. V. Chulkov, Low-coverage surface diffusion in complex periodic energy landscapes: Analytical solution for systems with symmetric hops and application to intercalation in topological insulators, *Phys. Rev. B* **93**, 075429 (2016).
DOI: 10.1103/PhysRevB.93.075429
2016 IF 3.836 (2016 18/67 Q2 T1 in Condensed Matter Physics).
Citations = 3 WS, 4 RG, 6 GS.
Theoretical derivation and computational validation of diffusivity formulae. Description of latest experiments on diffusion of metals on topological insulators.

2015:

12. H. Zhang, Y. Xing, M. A. Gosálvez, P. Pal, K. Sato, Removal probability function for Kinetic Monte Carlo simulations of anisotropic etching of silicon in alkaline etchants containing additives, *Sens. Actuator A-Phys.* **233** (2015) pp 451–459.
    DOI: 10.1016/j.sna.2015.07.031
    2015 IF 2.201 (1st class MEMS journal; 2015 58/257 Q1 T1 in Electrical & Electronic Engineering; 2015 44/850 Q1 T1 in Engineering).
    Citations = 2 WS, 3 RG, 5 GS.
13. Y. Li, M. A. Gosálvez, P. Pal, K. Sato and Y. Xing, Particle swarm optimization-based continuous cellular automaton for the simulation of deep reactive ion etching, *J. Micromech. Microeng*. **25** (2015) 055023 (13pp) DOI: 10.1088/0960-1317/25/5/055023
    2015 IF 1.768 (1st class MEMS journal; 2015 88/257 Q2 T2 in Electrical & Electronic Engineering; 2015 68/850 Q1 T1 in Engineering).
    Citations = 1 WS, 3 RG, 3 GS.
    Physical modeling + experiments.
14. Pal, Prem; Gosalvez, M. A.; Sato, Kazuo; Hida, H.; Xing, Yan, Erratum: Anisotropic etching on Si{110}: experiment and simulation for the formation of microstructures with convex corners, *J. Micromech. Microeng.* **25** 4 (2015) 049601 (1p).
    DOI: 10.1088/0960-1317/25/4/049601

2014:

15. Pal, Prem; Gosalvez, M. A.; Sato, Kazuo; Hida, H.; Xing, Yan, Anisotropic etching on Si{110}: experiment and simulation for the formation of microstructures with convex corners, *J. Micromech. Microeng.* **24** 12 (2014) 125001 (12pp).
    DOI: 10.1088/0960-1317/24/12/125001
    2014 IF 1.731 (1st class MEMS journal; 2014 85/249 Q2 T2 in Electrical & Electronic Engineering; 2014 65/838 Q1 T1 in Engineering).
    Citations = 5 WS, 6 RG, 8 GS.
    Accurate simulations.
16. N. Ferrando, M. A. Gosalvez, and A. Ayuela, Evolutionary Kinetic Monte Carlo - Atomistic Rates of Surface-Mediated Processes from Surface Morphologies, J. Phys. Chem. C, 2014, 118 (22), pp 11636–11648. DOI: 10.1021/jp409812x
    2014 IF 4.772 (2014 29/139 Q1 T1 in Physical Chemistry).
    Citations = 3 WS, 2 RG, 7 GS.
    Theory and simulation at the nanoscale. Extracting reactivity from morphology.
17. K. M. McPeak, C. D. van Engers, M. Blome, J. H. Park, S. Burger, M. A. Gosálvez, A. Faridi, Y.R. Ries, A. Sahu and D. J. Norris, Complex Chiral Colloids and Surfaces via High-Index Off-Cut Silicon, *Nano Letters*, 2014, 14 (5), pp 2934–2940.
    DOI: 10.1021/nl501032j
    2014 IF 13.592 (2014 8/157 Q1 T1 in Multidisciplinary Chemistry)
    Citations = 22 WS, 23 RG, 28 GS.
    Manufacture of chiral surface structures and particles with specific handedness using plasmonic metals. Record molar circular dichroism at red wavelengths and chiral

optical signatures resonant with biomolecules in the ultraviolet.

2013:

18. C. Montoliu, N. Ferrando, M. A. Gosálvez, J. Cerdá, R. J. Colom, Implementation and evaluation of the Level Set method: Towards efficient and accurate simulation of wet etching for microengineering applications, *Comput. Phys. Commun.* **184** (2013) 2299–2309.
    DOI: 10.1016/j.cpc.2013.05.016
    2013 IF 2.407 (2013 19/102 Q1 T1 in Interdisciplinary Applications of Computer Science)
    Citations = 9 WS, 8 RG, 15 GS.
    Implementation of accurate and efficient simulations. Fundamental for further improvements introduced into the "IntelliEtch" product (see C-3 above).
19. C. Montoliu, N. Ferrando, M. A. Gosálvez, J. Cerdá and R. J. Colom, Level set implementation for the simulation of anisotropic etching: application to complex MEMS micromachining, *J. Micromech. Microeng.* **23** (2013) 075017 (10pp).
    DOI: 10.1088/0960-1317/23/7/075017
    2013 IF 1.725 (1st class MEMS journal; 2013 79/248 Q2 T1 in Electrical & Electronic Engineering; 2013 63/837 Q1 T1 in Engineering).
    Citations = 6 WS, 6 RG, 7 GS.
    Accurate and efficient simulations.

2012:

20. B. Tang, K. Sato, M. A. Gosálvez, Sharp silicon tips with different aspect ratios in wet etching/DRIE and surfactant-modified TMAH etching, *Sens. Actuator A-Phys.* **188** (2012) 220–229. DOI: 10.1016/j.sna.2012.01.031
    2012 IF 1.841 (1st class MEMS journal; 2012 58/243 Q1 T1 in Electrical & Electronic Engineering; 2012 36/827 Q1 T1 in Engineering).
    Citations = 4 WS, 7 RG, 16 GS.
    Experimental.
21. Y. Xing, M. A. Gosálvez, K. Sato, M. Tian and H. Yi, Evolutionary determination of Kinetic Monte Carlo rates for the simulation of evolving surfaces in anisotropic etching of silicon, *J. Micromech. Microeng.* **22** (2012) 085020 (12pp).
    DOI: 10.1088/0960-1317/22/8/085020
    2012 IF 1.790 (1st class MEMS journal; 2012 65/243 Q2 T1 in Electrical & Electronic Engineering; 2012 56/827 Q1 T1 in Engineering).
    Citations = 6 WS, 7 RG, 12 GS.
    Theory. First proof of concept.
22. Prem Pal, M. A. Gosálvez, and K. Sato, Etched Profile Control in Anisotropic Etching of Silicon by TMAH+Triton, *J. Micromech. Microeng.* **22** (2012) 065013 (9pp).
    DOI: 10.1088/0960-1317/22/6/065013
    2012 IF 1.790 (1st class MEMS journal; 2012 65/243 Q2 T1 in Electrical & Electronic Engineering; 2012 56/827 Q1 T1 in Engineering).
    Citations = 10 WS, 14 RG, 22 GS.

Experiment and theory.

23. N. Ferrando, M. A. Gosálvez, R. J. Colóm, Evolutionary continuous cellular automaton for the simulation of wet etching of quartz, *J. Micromech. Microeng.* **22** (2012) 025021 (14pp). DOI: 10.1088/0960-1317/22/2/025021
2012 IF 1.790 (1st class MEMS journal; 2012 65/243 Q2 T1 in Electrical & Electronic Engineering; 2012 56/827 Q1 T1 in Engineering).
Citations = 10 WS, 14 RG, 18 GS.
Theory + applications. First atomistic simulator for wet etching of quartz.

2011:

24. M. A. Gosálvez, Prem Pal, N. Ferrando, K. Sato, Reliability assessment of the complete 3D etch rate distribution of Si in anisotropic etchants based on vertically micromachined wagon wheel samples, *J. Micromech. Microeng.* **21** (2011) 125008 (12pp). DOI: 10.1088/0960-1317/21/12/125008
2011 IF 2.105 (1st class MEMS journal; 2011 47/245 Q1 T1 in Electrical & Electronic Engineering). Citations = 2 WS, 10 RG, 5 GS.
Theory and modeling.
25. M. A. Gosálvez, Prem Pal, N. Ferrando, H. Hida, K. Sato, Experimental procurement of the complete 3D etch rate distribution of Si in anisotropic etchants based on vertically micromachined wagon wheel samples, *J. Micromech. Microeng.* **21** (2011) 125007 (14pp). DOI: 10.1088/0960-1317/21/12/125007
2011 IF 2.105 (1st class MEMS journal; 2011 47/245 Q1 T1 in Electrical & Electronic Engineering). Citations = 15 WS, 23 RG, 28 GS.
Experiment+theory+applications.
26. M. A. Gosálvez, Prem Pal, K Sato, Reconstructing the 3D etch rate distribution of silicon in anisotropic etchants using data from vicinal {100}, {110} and {111} surfaces, *J. Micromech. Microeng.* **21** (2011) 105018 (17pp).
DOI: 10.1088/0960-1317/21/10/105018
2011 IF 2.105 (1st class MEMS journal; 2011 47/245 Q1 T1 in Electrical & Electronic Engineering). Citations = 5 WS, 8 RG, 10 GS.
Theory.
27. M. A. Gosálvez, N. Ferrando, Y. Xing, Prem Pal, K. Sato, J. Cerdà, R. Gadea, Simulating anisotropic etching of silicon in any etchant: Evolutionary algorithm for the calibration of the continuous cellular automaton, *J. Micromech. Microeng.* **21** (2011) 065017 (15pp). DOI: 10.1088/0960-1317/21/6/065017
2011 IF 2.105 (1st class MEMS journal; 2011 47/245 Q1 T1 in Electrical & Electronic Engineering). Citations = 13 WS, 14 RG, 17 GS.
Article featured in 'Highlights Collection of 2011' by 'IOPselect' (Novelty, significance and potential impact on future research). Theory and simulation.
28. N. Ferrando, M. A. Gosálvez, J. Cerdà, R. Gadea, and K. Sato, Octree-based, GPU Implementation of a Continuous Cellular Automaton for the Simulation of Complex, Evolving Surfaces, *Comput. Phys. Commun.* **182** (2011) 628-640.
DOI: 10.1016/j.cpc.2010.11.004
2011 IF 3.268 (2011 10/99 Q1 T1 in Interdisciplinary Applications of Computer

Science)
Citations = 21 WS, 27 RG, 34 GS.
Computational implementation, markedly faster simulations.

29. N. Ferrando, M. A. Gosálvez, J. Cerdà, R. Gadea, and K. Sato, Faster and exact implementation of the Continuous Cellular Automaton for anisotropic etching simulations, *J. Micromech. Microeng.* **21** (2011) 025021 (15pp).
DOI: 10.1088/0960-1317/21/2/025021
2011 IF 2.105 (1st class MEMS journal; 2011 47/245 Q1 T1 in Electrical & Electronic Engineering). Citations = 4 WS, 5 RG, 6 GS.
Faster, accurate simulations. Theory and computation.
30. P. Pal, M. A. Gosálvez, K. Sato, B. Tang, H. Hida, and M. Shikida, Fabrication of novel microstructures based on orientation dependent adsorption of surfactant molecules in a TMAH solution, *J. Micromech. Microeng.* **21** (2011) 015008 (11pp).
DOI: 10.1088/0960-1317/21/1/015008
2011 IF 2.105 (1st class MEMS journal; 2011 47/245 Q1 T1 in Electrical & Electronic Engineering). Citations = 19 WS, 24 RG, 29 GS.
Experiment and theory.

2010:

31. P. Pal, M. A. Gosálvez, and K. Sato, Silicon Micromachining Based on Surfactant-Added Tetramethyl Ammonium Hydroxide: Etching Mechanism and Advanced Applications, *Jpn. J. Appl. Phys.* **49** (2010) 056702 (9pp).
DOI: 10.1143/JJAP.49.056702
2010 IF 1.024 (2010 76/125 Q3 T2 in Applied Physics)
Citations = 18 WS, 22 RG, 25 GS.
Physical modeling, advanced technological applications.
32. M. A. Gosálvez,Y. Xing, K. Sato, and R. M. Nieminen, Octree-Search Kinetic Monte Carlo, *Sens. Actuator A-Phys.* **159** (2010) 64-68. DOI: 10.1016/j.sna.2010.02.003
2010 IF 1.941 (1st class MEMS journal; 2010 47/247 Q1 T1 in Electrical & Electronic Engineering).
Citations = 3 WS, 3 RG, 4 GS.
Computational method.
33. M. A. Gosálvez, P. Pal, B. Tang, and K. Sato, Letter to the Editor - Atomistic mechanism for the macroscopic effects induced by small additions of surfactants to alkaline etching solutions, *Sens. Actuator A-Phys.* **157** (2010) 91-95.
DOI: 10.1016/j.sna.2009.10.023
2010 IF 1.941 (1st class MEMS journal; 2010 47/247 Q1 T1 in Electrical & Electronic Engineering).
Citations = 11 WS, 15 RG, 18 GS.
Physical modeling, experiment.
34. Y. Xing, M. A. Gosálvez, K. Sato, and H Yi, Orientation-dependent surface morphology of crystalline silicon during anisotropic etching using a Continuous Cellular Automaton, *J. Micromech. Microeng.* **20** (2010) 015019 (11pp).DOI: 10.1088/0960-1317/20/1/015019

2010 IF 2.281 (1st class MEMS journal; 2010 33/247 Q1 T1 in Electrical & Electronic Engineering). Citations = 5 WS, 7 RG, 7 GS.

Theory and simulation.

2009:

35. B. Tang, P. Pal, M. A. Gosálvez, M. Shikida, K. Sato, H. Amakawa, and S. Itoh, Ellipsometry study of the adsorbed surfactant thickness on Si{110} and Si{100} and the effect of pre-adsorbed surfactant layer on etching characteristics in TMAH, *Sens. Actuator A-Phys.* **156** (2009) 334-341.
DOI: 10.1016/j.sna.2009.10.017
2009 IF 1.674 (1st class MEMS journal; 2009 65/246 Q2 T1 in Electrical & Electronic Engineering).
Citations = 25 WS, 30 RG, 39 GS.
36. M. A. Gosálvez, B. Tang, P. Pal, K. Sato, Y. Kimura, K. Ishibashi, Orientation- and concentration-dependent surfactant adsorption on silicon in aqueous alkaline solutions: explaining the changes in the etch rate, roughness and undercutting for MEMS applications, *J. Micromech. Microeng.* **19** (2009) 125011 (18pp).
DOI: 10.1088/0960-1317/19/12/125011
2009 IF 1.997 (1st class MEMS journal; 2009 43/246 Q1 T1 in Electrical & Electronic Engineering). Citations = 36 WS, 47 RG, 57 GS.
Theory, simulation and experiment.
Experimental study and theoretical model.
37. M. A. Gosálvez,Y. Xing, K. Sato, and R. M. Nieminen, Discrete and continuous cellular automata for the simulation of propagating surfaces, *Sens. Actuator A-Phys.* **155** (2009) 98-112.
DOI: 10.1016/j.sna.2009.08.012
2009 IF 1.674 (1st class MEMS journal; 2009 65/246 Q2 T1 in Electrical & Electronic Engineering).
Citations = 13 WS, 16 RG, 25 GS.
Computational modeling. Comparison of pros and cons of two methods.
38. P. Pal, K. Sato, M. A. Gosálvez, Y. Kimura, K. Ishibashi, M. Niwano, H. Hida, B. Tang, and S. Itoh, Surfactant Adsorption on Single Crystal Silicon Surfaces in TMAH Solution: Orientation-Dependent Adsorption Detected by In-situ Infra-Red Spectroscopy, *J. Microelectromech. Syst.* **18** (2009) 1345-1356.
DOI: 10.1109/JMEMS.2009.2031688
2009 IF 1.922 (1st class MEMS journal; 2009 9/116 Q1 T1 in Mechanical Engineering ; 2009 49/246 Q1 T1 in Electrical & Electronic Engineering).
Citations = 36 WS, 41 RG, 47 GS.
Experimental measurements and physical modeling.
39. P. Pal, K. Sato, M. Shikida, and M. A. Gosálvez, Study of corner compensating structures and fabrication of various shapes of MEMS structures in pure and surfactant added TMAH, *Sens. Actuator A-Phys*. **154** (2009) 192-203.
DOI: 10.1016/j.sna.2008.09.002
2009 IF 1.674 (1st class MEMS journal; 2009 65/246 Q2 T1 in Electrical &

Electronic Engineering).
Citations = 40 WS, 50 RG, 66 GS.
Experimental study.

2008:

40. T. Hynninen and M. A. Gosálvez, Model for hydrogen bubbles and connection to roughness of etched surfaces, *J. Chem. Phys.* **129** (2008) 156101 (2pp).
DOI: 10.1063/1.2996514
2008 IF 3.149 (2008 5/31 Q1 T1 in Atomic, Molecular & Chemical Physics)
Citations = 0 WS, 3 RG, 6 GS.
Chemistry.
41. T. Hynninen, A. S. Foster, M. A. Gosálvez, R. M. Nieminen, and K. Sato, Adsorption of metal impurities on H-terminated Si surfaces and their effect on wet etching of Si, *J. Phys.-Condens. Matter* **20** (2008) 485005 (9pp).
DOI: 10.1088/0953-8984/20/48/485005
2008 IF 1.900 (2008 17/62 Q2 T1 in Condensed Matter Physics)
Citations = 3 WS, 5 RG, 4 GS.
Combines ab-initio DFT calculations for adsorption/desorption energetics and KMC simulations for mesoscopic kinetics.
42. M. A. Gosálvez, Y. Xing, and K. Sato, Analytical solution of the Continuous Cellular Automaton for anisotropic etching, *J. Microelectromech. Syst.* **17** (2008) 410-431.
DOI: 10.1109/JMEMS.2008.916339
2008 IF 2.226 (1st class MEMS journal; 2008 6/105 Q1 T1 in Mechanical Engineering ; 2008 46/229 Q1 T1 in Electrical & Electronic Engineering).
Citations = 32 WS, 38 RG, 40 GS.
Theory, computational modeling.
43. M. A. Gosálvez, Y. Xing, K. Sato, and R. M. Nieminen, Atomistic methods for the simulation of evolving surfaces, *J. Micromech. Microeng.* **18** (2008) 055029 (17pp).
DOI: 10.1088/0960-1317/18/5/055029
2008 IF 2.233 (1st class MEMS journal; 2008 44/229 Q1 T1 in Electrical & Electronic Engineering). Citations = 22 WS, 23 RG, 37 GS.
Article featured in 'Highlights Collection of 2008' by 'IOPselect' (Novelty, significance and potential impact on future research). Review. Computational modeling.
44. T. Hynninen, M. A. Gosálvez, A. S. Foster, R. M. Nieminen, H. Tanaka, K. Sato, and M. Uwaha, Effect of Cu impurities on wet etching of Si(110): formation of trapezoidal hillocks, *New J. Phys.* **10** (2008) 013033 (19pp).
DOI: 10.1088/1367-2630/10/1/013033
2008 IF 3.440 (2008 9/68 Q1 T1 in Multidisciplinary Physics)
Citations = 6 WS, 8 RG, 10 GS. Surface science. Physics.

2007:

45. Y. Xing, M. A. Gosálvez, and K. Sato, Step flow based Cellular Automaton for the simulation of anisotropic etching of complex MEMS structures, *New J. Phys.* **9** (2007) 436 (18pp). DOI: 10.1088/1367-2630/9/12/436

2007 IF 3.264 (2007 10/69 Q1 T1 in Multidisciplinary Physics)
Citations = 28 WS, 31 RG, 40 GS. Computational.

46. P. Pal, K. Sato, M. A Gosálvez, and M. Shikida, Study of rounded concave and sharp edge convex corners undercutting in CMOS compatible anisotropic etchants, *J. Micromech. Microeng.* **17** (2007) 2299–2307.
DOI: 10.1088/0960-1317/17/11/017
2007 IF 1.930 (1st class MEMS journal; 2007 29/227 Q1 T1 in Electrical & Electronic Engineering). Citations = 31 WS, 49 RG, 56 GS.
Technological applications.
47. A. S. Foster, M. A. Gosálvez, T. Hynninen, R. M. Nieminen, and K. Sato, First-principles calculations of Cu adsorption on an H-terminated Si surface, *Phys. Rev. B* **76** (2007) 075315 (8pp). DOI: 10.1103/PhysRevB.76.075315
2007 IF 3.172 (2007 9/61 Q1 T1 in Condensed Matter Physics)
Citations = 11 WS, 14 RG, 18 GS. Physics and chemistry.
48. M. A. Gosálvez, Y. Xing, T. Hynninen, M. Uwaha, A. S. Foster, R. M. Nieminen, and, K. Sato, Faster simulations of step bunching during anisotropic etching: formation of zigzag structures on Si(110), *J. Micromech. Microeng.* **17** (2007) S27–S37.
DOI: 10.1088/0960-1317/17/4/S02
2007 IF 1.930 (1st class MEMS journal; 2007 29/227 Q1 T1 in Electrical & Electronic Engineering). Citations = 13 WS, 15 RG, 20 GS.
Computational physics.
49. M. A. Gosálvez, K. Sato, A. S. Foster, R. M. Nieminen, and H. Tanaka, An atomistic introduction to anisotropic etching, *J. Micromech. Microeng.* **17** (2007) S1-S26.
DOI: 10.1088/0960-1317/17/4/S01
2007 IF 1.930 (1st class MEMS journal; 2007 29/227 Q1 T1 in Electrical & Electronic Engineering). Citations = 67 WS, 74 RG, 101 GS.
Review.

2006:

50. J. Werkmeister, M. A. Gosálvez, P. Willoughby, A. Slocum and K. Sato, Anisotropic Etching of Silicon as a Tool for Creating Injection Molding Tooling Surfaces, *J. Microelectromech. Syst.* **15** (2006) No. 6, 1671-1680.
DOI: 10.1109/JMEMS.2006.885989
2006 IF 2.659 (1st class MEMS journal; 2006 6/106 Q1 T1 in Mechanical Engineering ; 2008 11/206 Q1 T1 in Electrical & Electronic Engineering).
Citations = 7 WS, 7 RG, 10 GS.
Experimental and computational modeling.
51. M. A. Gosálvez, D. Cheng, R. M. Nieminen and K. Sato, Apparent activation energy during surface evolution by step formation and flow, *New J. Phys.* **8** (2006) 269 (11pp).
DOI: 10.1088/1367-2630/8/11/269
2006 IF 3.754 (2006 9/68 Q1 T1 in Multidisciplinary Physics)
Citations = 12 WS, 14 RG, 14 GS. Theoretical physics.
52. D. Cheng, M. A. Gosálvez, T. Hori, K. Sato and M. Shikida, Improvement in smoothness of anisotropically etched silicon surfaces: Effects of surfactant and TMAH

concentrations, *Sens. Actuator A-Phys.* **125** (2006) 415-421.
DOI: 10.1016/j.sna.2005.08.022
2006 IF 1.434 (1st class MEMS journal; 2006 44/206 Q1 T1 in Electrical & Electronic Engineering).
Citations = 44 WS, 54 RG, 62 GS.
Physics / MEMS.

2005-2001:

53. Gosálvez M. A., Nieminen R. M. and K. Sato, Arrhenius and non-Arrhenius behaviour during anisotropic etching, *Sensors and Materials* **17** (2005) No. 4, 187-197.
ISSN: 0914-4935
2014 IF 0.450 (2005 121/178 Q3 T3 in Multidisciplinary Materials Science)
Citations = 2 WS, 3 RG, 0 GS. Theory / Physics.
http://myukk.org/Vol17-4.html
54. Gosálvez M. A. and Nieminen R. M., Target-Rate Kinetic Monte Carlo Method for Simulation of Nanoscale Structural Evolution, *J. of Computational and Theoretical Nanoscience* **1** (2004) No. 3, 303-308. DOI: 10.1166/jctn.2004.032
2015 IF 1.666 (2015 84/163 Q3 T2 in Multidisciplinary Chemistry)
Citations = 0 WS, 1 RG, 1 GS. Computational topic.
55. Gosálvez M. A. and Nieminen R. M., Relation between macroscopic and microscopic activation energies in non-equilibrium surface processing, *Phys. Rev. E* **68** (2003) 031604 (16pp). DOI: 10.1103/PhysRevE.68.031604
2013 IF 2.202 (2003 1/31 Q1 T1 in Mathematical Physics)
Citations = 4 WS, 4 RG, 8 GS. Surface processing. Physics.
56. Gosálvez M. A. and Nieminen R. M., Surface morphology during anisotropic wet chemical etching of crystalline silicon, *New J. Phys.* **5** (2003) 100.1-100.28.
DOI: 10.1088/1367-2630/5/1/400
2003 IF 2.480 (2003 10/68 Q1 T1 in Multidisciplinary Physics)
Citations = 56 WS, 65 RG, 103 GS.
Surface processing. Surface morphology. Physics.
57. Gosálvez M. A., Foster A. S. and Nieminen R. M., Dependence of the anisotropy of wet chemical etching of silicon on the amount of surface coverage by OH radicals, *Sensors and Materials* **15** (2003) 53-65.
2014 IF 0.450 (2003 89/177 Q3 T2 in Multidisciplinary Materials Science)
Citations = 3 WS, 3 RG, 4 GS. Theoretical / Computational topic.
58. Gosálvez M. A., Foster A. S. and Nieminen R. M., Atomistic simulations of surface coverage effects in anisotropic wet chemical etching of crystalline silicon, *Applied Surface Science* **202** (2002) 160-182.
DOI: 10.1016/S0169-4332(02)00903-0
2002 IF 1.295 (2002 25/71 Q2 T2 in Applied Physics)
Citations = 33 WS, 40 RG, 47 GS. Computational modeling.
59. Gosávez M. A., Foster A. S. and Nieminen R. M., Multiscale modeling of anisotropic wet chemical etching of crystalline silicon, *Europhysics Letters* **60** (2002) 467-473.
DOI: 10.1209/epl/i2002-00287-1

2002 IF 2.360 (2002 9/68 Q1 T1 in Multidisciplinary Physics)
Citations = 15 WS, 13 RG, 22 GS. Computational modeling.

60. Gosálvez M. A., Nieminen R. M., Kilpinen P., Haimi E. and Lindroos V., Anisotropic wet chemical etching of crystalline silicon: atomistic Monte-Carlo simulations and experiments, *Applied Surface Science* **178** (2001) 7-26.
DOI: 10.1016/S0169-4332(01)00233-1
2001 IF 1.068 (2001 29/71 Q2 T2 in Applied Physics)
Citations = 45 WS, 43 RG, 63 GS. Computational physics.

Papers in peer-reviewed proceedings of international conferences: (24)

1. J. Zhang, Y. Xing, M. A. Gosálvez, Xiaoli Qiu, Xiaohui Lin, Chibin Zhang, Level Set Simulation of Surface Evolution in Anisotropic Wet Etching of patterned Sapphire Substrate, The 32nd IEEE International Conference on Micro Electro Mechanical Systems (MEMS 2019), January 27-31 2019, Coex, Seoul, South Korea. (Poster W-021) **[Citations = 0 WS, 0 RG, 0(GS)]** DOI: Not yet available as of May 2019.
2. Y. Xing, Z. Guo, G. Wu, M. A. Gosalvez, Characterization of orientation-dependent etching properties and surface morphology of sapphire crystal in wet etching, The 20th International Conference on Solid-State Sensors, Actuators and Microsystems (Transducers 2019 - EUROSENSORS XXXIII), 23-27 June 2019, Berlin, Germany (Oral T2E.002) **[Citations = 0 WS, 0 RG, 0(GS)]** DOI: Not yet available as of May 2019.
3. Y Zhang, J Zhang, Y Xing, H Zhang, M A Gosálvez, X Qiu, The level set simulation for complex microstructures in quartz wet etching, In Proc. of the 19th International Conference on Solid-State Sensors, Actuators and Microsystems (Transducers 2017), 18-22 June 2017, Kaohsiung, Taiwan. pp. 1356-1359 (Poster W3P.035) **[Citations = 0 WS, 0 RG, 0(GS)]** DOI: 10.1109/TRANSDUCERS.2017.7994308
4. H Zhang, Y Xing, J Zhang, M A Gosálvez, Y Li, Y Zhang, Evolutionary Kinetic Monte Carlo method for the simulation of anisotropic etching of Z-cut, AT-cut and BT-cut quartz, In Proc. of the 19th International Conference on Solid-State Sensors, Actuators and Microsystems (Transducers 2017), 18-22 June 2017, Kaohsiung, Taiwan. pp. 1308-1311 (Poster M3P.034) **[Citations = 0 WS, 0 RG, 0(GS)]** DOI: 10.1109/TRANSDUCERS.2017.7994296
5. M. A. Gosálvez, Y. Zhou, Y. Zhang, G. Zhang, Y. Li and Y. Xing, Simulation of microloading and ARDE in DRIE, In Proc. of the 18th International Conference on Solid-State Sensors, Actuators and Microsystems (Transducers 2015), June 21-25, 2015, Anchorage, Alaska, USA. pp. 1255-1258 (Poster M3P.019) **[Citations = 0 WS, 0 RG, 0(GS)]** DOI: 10.1109/TRANSDUCERS.2015.7181158
6. Y. Li, Y. Xing, M. A. Gosálvez, Prem Pal and Y. Zhou, Particle Swarm Optimization of Model Parameters: Simulation of Deep Reactive Ion Etching by the Continuous Cellular Automaton, In Proc. of the 17th International Conference on Solid-State Sensors, Actuators and Microsystems (Transducers 2013), June16-20, 2013, Barcelona, Spain. (Poster T3P.043) **[Citations = 0 WS, 1 RG, 2(GS)]**
DOI: 10.1109/Transducers.2013.6626960

7. C. Montoliu, N. Ferrando, J. Cerdá, R. J. Colom and M. A. Gosálvez, Application of the Level Set Method for the Visual Representation of Continuous Cellular Automata Oriented to Anisotropic Wet Etching, Editors: L. Jódar, L. Acedo, J. C. Cortés and F. Pedroche, In Proc. of international conference on Modelling for Engineering & Human Behaviour 2012, Instituto Universitario de Matemática Multidisciplinar, Polytechnic City of Innovation, Valencia, Spain, Sep 4-7, 2012, 5 pages (Oral, talk number 24). DOI:10.1080/00207160.2013.801464
8. Prem Pal, M. A. Gosálvez, and K. Sato, Dependence of undercutting on stirring and galvanic interactions between emerging facets during silicon etching in TMAH+Surfactant, The Sixth Asia-Pacific Conference on Transducers and Micro/Nano Technologies, IEEE APCOT 2012, July 8-11, 2012, Nanjing, China, 2 pages (Poster ac12000166).
9. Y. Xing, M. A. Gosálvez, K. Sato, and M. Tian, A genetic algorithm based kinetic Monte Carlo simulation for the evolution of complex surface in anisotropic wet etching, in *Proc. of Transducers 2011 - The 16th Intl. Conference on Solid-State Sensors, Actuators and Microsystems*, June 5-9, 2011, Beijing, China, 2 pages (Poster 06-039) **[Citations = 0 WS, 2 RG, 3 GS]** DOI: 10.1109/TRANSDUCERS.2011.5969477
10. B. Tang, K. Sato, H. Tanaka and M. A. Gosálvez, Fabrication of sharp tips with high aspect ratio by surfactant-modified wet etching for the AFM probe, in *Proc. MEMS 2011*, The *24th International Conference on Micro Electro Mechanical Systems,* January 23 - 27, 2011, Cancun, Mexico, p. 328-331 (Poster) **[Citations = 3 WS, 5 RG]** DOI: 10.1109/MEMSYS.2011.5734428
11. Prem Pal, K. Sato, M. A. Gosálvez, B. Tang and H. Hida, Advanced MEMS Applications using Orientation Dependent Adsorption of Surfactant Molecules in TMAH Solution, The 5th Asia-Pacific Conference on Transducers and Micro-Nano Technology (APCOT 2010), Jul. 6-9, 2010, Perth, Western Australia, FT13, p. 79 (Oral)
12. B. Tang, M. A. Gosálvez, P. Pal, S. Itoh, H. Hida, M. Shikida, and K. Sato, Adsorbed Surfactant Thickness on a Si Wafer Dominating Etching Properties of TMAH Solution, IEEE Intl. Conf. on MHS 2009 & Micro-Nano Global COE, The 2009 International Symposium on Micro-Nano Mechatronics and Human Science, Nov. 8-11, 2009, Nagoya, Japan, p. 48-52 (Poster P1-7) **[Citations = 0 WS, 2 RG, 1 GS]** DOI: 10.1109/MHS.2009.5352098
13. M. A. Gosálvez, Y. Xing and K. Sato, Continuous Cellular Automaton for the propagation of advancing fronts featuring surface morphologies: Realistic simulation of wet etching for MEMS applications, IEEE Intl. Conf. on MHS 2009 & Micro-Nano Global COE, The 2009 International Symposium on Micro-Nano Mechatronics and Human Science, Nov. 8-11, 2009, Nagoya, Japan, 2 pages (Poster P1-50) DOI: 10.1109/SENSOR.2009.5285587
14. P. Pal, K. Sato, M. A. Gosálvez, Y. Kimura, K. Ishibashi, M. Niwano, H. Hida, B. Tang, and S. Itoh, Experimental Verification and Theoretical Explanation of the Effect of Surfactant Addition to TMAH Based Etchants for Advanced Applications in MEMS, IEEJ SMS Symposium on Sensors, Micromechanics and Applied Systems, Tokyo, Japan, October 15-16, 2009, p. 150-154 (Poster)
15. N. Ferrando, J. Cerdà, M. A. Gosálvez and J. D. Martinez, Performing Fast Anisotropic

Wet Etching Simulations by Using Graphic Processing Units, in *Proc. of MME 2009 - The 20th Workshop on Micromachining, Micromechanics and Microsystems*, Sep 20-22, 2009, Toulouse, France, Paper ID: 123, 4 pages (Oral)

16. Y. Xing, M. A. Gosálvez, and K. Sato, Continuous Cellular Automaton for the simulation of the surface morphology on any silicon orientation Si{hkl} in anisotropic etching, in *Proc. of Transducers 2009 - The 15th Intl. Conference on Solid-State Sensors, Actuators and Microsystems*, June 21-25, 2009, Denver, Colorado, USA, p. 747-750 (Oral, by M. A. Gosálvez) **[Citations = 0 WS, 1 RG, 0 GS]**
DOI: 10.1109/SENSOR.2009.5285587.
17. P. Pal, K. Sato, H. Hida, M. A. Gosálvez, Y. Kimura, K. Ishibashi and M. Niwano, Surfactant in TMAH for new shapes of silicon MEMS components; Its orientation dependent adsorption detected by infrared spectroscopy, in *Proc. of Transducers 2009 - The 15th Intl. Conference on Solid-State Sensors, Actuators and Microsystems*, June 21-25, 2009, Denver, Colorado, USA, p.751-754 (Oral) **[Citations = 1 GS]**
DOI: 10.1109/SENSOR.2009.5285602
18. Y. Xing, M. A. Gosálvez, and K. Sato, A Continuous Cellular Automaton for the Atomistic Simulation of Evolving Surface in Anisotropic Etching, Fourth International Conference on Natural Computation, ICNC, vol. 7, 2008, p.402-406, Jinan, Shandong, China, 18-20 October, 2008. (Oral) DOI: 10.1109/ICNC.2008.237 **[Citations = 1 GS]**
19. M. A. Gosálvez, VisualTAPAS: an example of DFT-assisted understanding and simulation of anisotropic etching, in 'Theory Meets Industry', June 12-14, 2007, Erwin-Schrdinger-Institute for Mathematical Physics, Wien, Austria. *J. Phys.-Condens. Matter* **20** (2008) 064234. (Oral) **[Citations = 2 GS]**
DOI: 10.1088/0953-8984/20/6/064234
20. P. Pal, K. Sato, M.A. Gosálvez and M. Shikida, An improved anisotropic wet etching process for the fabrication of silicon MEMS structures using a single etching mask, in *Proc. of MEMS 2008, The 21st IEEE International Conference on Micro Electro Mechanical Systems*, Jan. 13-17, 2008, Tucson, USA, p. 327-230 (Poster) **[Citations = 5 WS, 5 GS]** DOI: 10.1109/MEMSYS.2008.4443659
21. Y. Xing, M. A. Gosálvez, and K. Sato, Octree-search Kinetic Monte Carlo algorithm for the simulation of complex 3D MEMS structures, in *Proc. of MEMS 2008, The 21st IEEE International Conference on Micro Electro Mechanical Systems*, Jan. 13-17, 2008, Tucson, Arizona, USA, p. 323-326 (Poster) **[Citations = 2 WS, 7 GS]**
DOI: 10.1109/MEMSYS.2008.4443658
22. P. Pal, K. Sato, M. A. Gosálvez and M. Shikida, Microstructures with rounded concave and sharp-edged convex corners in a single step wet anisotropic etching, in *Proc. of MEOMS-MEMS 2008 (part of SPIE Photonics West 2008)*, Jan 19-24, 2008, San Jose Convention Center, San Jose, California, USA, Proc. of SPIE Vol. 6882 (2008) p. 68820F-1-8 (Oral) DOI: 10.1117/12.765475 **[Citations = 1 GS]**
23. P. Pal, K. Sato, M. A. Gosálvez, M. Shikida, Novel wet anisotropic etching process for the realization of new shapes of silicon MEMS structures, *IEEE Intl. Conf. on MHS 2007 & Micro-Nano COE, The 2007 International Symposium on Micro-Nano Mechatronics and Human Science*, Nov. 12-14, 2007, Nagoya, Japan, p. 499-504 (Poster) **[Citations = 1 WS, 4 GS]** DOI: 10.1109/MHS.2007.4420906

24. D. Cheng, M. A. Gosálvez, M. Shikida and K. Sato, A universal parameter for silicon anisotropic etching in alkaline solutions, in *Proc. MEMS 2006*, The *19th IEEE International Conference in Micro Electro Mechanical Systems,* Jan 22-26, 2006, Istanbul, Turkey, p. 318-321 (Oral) **[Citations = 3 GS]**
DOI: 10.1109/MEMSYS.2006.1627800

Presentations in international meetings and workshops: (26)

1. M. A. Gosálvez, J. Alberdi-Rodriguez, 'Another approach to heterogeneous catalysis', Division of Catalysis Science and Technology, ACS Spring 2019 National Meeting, Session in 'Advances in Methods for Comparing Molecular & Supramolecular Simulations to Experiments', Orange County Convention Center, Orlando, Florida, USA, March, 31, 2019. (Oral)
2. M Otrokov, A Ryabishchenkova, MA Gosalvez, V Kuznetsov, E Chulkov, Ab initio study of the adsorption, diffusion, and intercalation of alkali metal atoms on the (0001) surface of the topological insulator Bi2 Se3, APS Meeting Abstracts, APS March Meeting 2016, March 14-18, 2016, Baltimore, MD, U.S.A. (Oral)
3. A.G. Ryabishchenkova, M.M. Otrokov, M.A. Gosalvez, V. Kuznetsov, and E.V. Chulkov, Adsorption, diffusion and intercalation of alkali metal atoms deposited on the stepped Bi2Se3 surface: an ab initio study, The 7th International Symposium on Surface Science (ISSS-7), Shimane Prefectural Convention Center, Kunibiki Messe, Matsue, Shimane, Japan, Nov. 2 - 6, 2014, 1p (Oral, 4pA2-2)
4. M. A. Gosálvez, "Evokinetics: A software tool for the analysis of CVD growth of novel 2D materials?", 14th edition of Trends in Nanotechnology International Conference (TNT 2013), Sevilla, Spain, Sep 9-13, 2013. (Oral)
5. M. A. Gosálvez, Atomistic simulations of anisotropic etching, Baskrete Industry Open Days, Donostia International Physics Center DIPC, Donostia - San Sebastián, Spain, March 12-13, 2012. (Oral)
6. N. Ferrando and M. A. Gosálvez, Atomistic model for the simulation of anisotropic wet etching of Quartz, 1st NanoIKER Workshop, CIC NanoGune, Donostia - San Sebastián, Spain, March 12, 2012 (Poster P6)
7. M. A. Gosálvez, "Reliable atomistic simulations of anisotropic etching for MEMS applications", MEMS for personal life, Nagoya University, Nagoya, Japan, March 1-2, 2012 (Invited oral)
8. M. A. Gosálvez, "New features in IntelliEtch", IntelliSense Workshop, Jiangsu IntelliSense Technology Co., Ltd., Nanjing, China, June 11-12, 2011. (Oral)
9. T. Hynninen, M. A. Gosálvez, A. S. Foster, K. Sato, R. M. Nieminen, Effect of metal impurities on the surface morphology of wet etched Si, Conference "Physics Days 2009", Annual meeting by the Finnish Physical Society, Dipoli conference center, Otaniemi, Espoo, Helsinki area, Finland, March 12-14, 2009. (Oral) **[C = 0 GS]**
10. K. Sato, M. Shikida, M.A. Gosálvez and Prem Pal, Micro/Nano science uncovering the mysteries of silicon wet etching for the fabrication of MEMS structures, ICMAT (Intl. Conf. on Materials for Advanced Technologies) and IUMRS-ICA (Intl. Union of Materials Research Societies- Intl. Conf. in Asia), Singapore, 28 June - 3 July, 2009,

#A20613-04466 (Oral, invited)

11. Gosálvez M. A., VisualTAPAS: an example of DFT-assisted understanding and simulation of anisotropic etching, in 'Theory Meets Industry', June 12-14, 2007, Erwin-Schrodinger-Institute for Mathematical Physics, Wien, Austria. J. Phys.-Condens. Matter 20 (2008) 064234. (Oral, invited)
12. M. A. Gosálvez, Atomististic simulation of anisotropic etching, in 'Towards Reality in Nanoscale Materials', December 10-12, 2007, Levi, Finland. (Invited)
13. R. M. Nieminen, M. A. Gosálvez, and K. Sato, TAPAS: Three-dimensional Anisotropic Processing at All Scales, China, Summer 2007. (Oral, invited)
14. M. A. Gosálvez, Towards a simplified theoretical model for anisotropic etching: experimental aspects and realistic simulations, *First International Workshop on 'Progress in anisotropic wet chemical etching' (PiAWCE)*, Nov. 30 - Dec. 1st, 2006, Levi, Finland (www.fyslab.hut.fi/~tjh/workshop.html) (Oral)
15. Y. Xing, M. A. Gosálvez, and K. Sato, An efficient octree-topology based atomistic simulator of anisotropic etching, *First International Workshop on 'Progress in anisotropic wet chemical etching' (PiAWCE)*, Nov. 30 - Dec. 1, 2006, Levi, Finland (www.fyslab.hut.fi/~tjh/workshop.html) (Oral)
16. T. Hynninen, A. S. Foster, M. A. Gosálvez, H. Tanaka, R. M. Nieminen, and K. Sato, Role of metal impurities in anisotropic wet chemical etching of silicon, *First International Workshop on 'Progress in anisotropic wet chemical etching' (PiAWCE)*, Nov. 30 - Dec. 1, 2006, Levi, Finland (www.fyslab.hut.fi/~tjh/workshop.html) (Oral)
17. T. Hynninen, A. S. Foster, M. A. Gosálvez, H. Tanaka, R. M. Nieminen, K. Sato, Role of Metal Impurities in Anisotropic Wet Chemical Etching, *Proc. of AVS 53rd International Symposium*, November 13, 2006, San Francisco, USA. (Oral)
18. M. A. Gosálvez, Y. Xing, T. Hynninen, M. Uwaha, A. S. Foster, and R. M. Nieminen, and K. Sato, Formation of zigzag structures on anisotropically etched Si(110), in *Proc. of Symposium on 'Micro- and Nano-Mechatronics for Information-Based Society' of The 21st Century COE Program, MHS2006 & Micro-Nano COE*, Nagoya University, Nov. 5-8, 2006, Nagoya, Japan, 2 pages (Poster P2-14)
    http://www.mein.nagoya-u.ac.jp/mhs/MHS2006-Top.html
19. M. A. Gosálvez, An atomistic introduction to anisotropic etching, in Proc. of *The Fifth International Workshop on Physical Chemistry of Wet Etching of Semiconductors, PCWES 2006*, June 19-21, 2006, Saarbrucken, Germany, p. 1-7 (Oral, invited)
20. Y. Xing, M. A. Gosálvez, T. Hynninen, K. Sato, A. S. Foster, R. M. Nieminen, Fast step bunching method for surface morphology simulations of anisotropic etching, in *Proc. of The Fifth International Workshop on Physical Chemistry of Wet Etching of Semiconductors, PCWES 2006*, June 19 - 21, 2006, Saarbrücken, Germany, p. 61-65. (Oral, by M. A. Gosálvez)
21. M. A. Gosálvez, D. Cheng, R. M. Nieminen, K. Sato, Apparent activation energy of the etch rate in the vicinity of Si (111), in *Proc. of The Fifth International Workshop on Physical Chemistry of Wet Etching of Semiconductors*, *PCWES 2006*, June 19 - 21, 2006, Saarbrücken, Germany, p. 14-15 (Oral)
22. M. A. Gosálvez, J. Werkmeister, P. Willoughby, A. Slocum and K. Sato, Wet etched silicon inserts for injection molding, in *Proc. of Symposium on 'Micro- and Nano-*

Mechatronics for Information-Based Society' of The 21st Century COE Program, MHS2005 & Micro-Nano COE, Nov. 8-9, 2005, Nagoya, Japan, 2 pages (Poster P18) http://www.mein.nagoya-u.ac.jp/mhs/MHS2005-Top

23. M. A. Gosálvez and K. Sato, Exploring the activation energy during nanoscale structural evolution in wet etching, in *Proc. of Symposium on 'Micro- and Nano-Mechatronics for Information-Based Society' of The 21st Century COE Program, MHS2004 Micro-Nano COE*, Oct 31 – Nov 3, 2004, Nagoya, Japan, p. 127-132 (Oral). **[Citations = 0 GS]**
24. Gosálvez M. A., Nieminen R. M. and K. Sato, Arrhenius and non-Arrhenius behaviour during anisotropic etching, in Proc. of PCWES 2004, The 4th Workshop on Physical Chemistry of Wet Etching of Silicon, May 26-28, 2004, Montreal, Canada, 6 pages (Oral)
25. Gosálvez M. A., Foster A. S. and Nieminen R. M., Atomistic simulations of surface coverage effects in anisotropic wet chemical etching of crystalline silicon, in Proc. of PCWES 2002*, The 3rd Workshop on Physical Chemistry of Wet Etching of Silicon* (Nara, Japan, June 2002), Ed. K. Sato, p. 37-40. (Oral)
26. Gosálvez M. A., Foster A. S. and Nieminen R. M., Combining Monte Carlo Simulations and Ab-initio Calculations in Understanding of Wet Chemical Etching of Si, E-MRS Spring Meeting 2001, Symposium A, Computational Materials Science Across Time and Length Scales, June 5 - 8, 2001. (Oral)

Oral presentations during collaboration visits (from 2009): (11)

1. M. A. Gosálvez, Simulating surface processing with evolutionary atomistic methods for microengineering applications, School of Chemistry, University of St Andrews, St Andrews, Fife, KY16 9ST, Scotland, UK, May 22, 2012.
2. M. A. Gosálvez, Surface processing simulations by evolutionary atomistic methods for microengineering applications, Nano group, Faculty of Applied Physical Science, Southampton University, United Kingdom, May 18, 2012.
3. M. A. Gosálvez, "Reliable atomistic simulations of anisotropic etching for MEMS applications", College of Electronic and Information Engineering, Nanjing University of Information Science and Technology, Nanjing, China, March 9, 2012.
4. M. A. Gosálvez, "Experimental characterization of spray etching of copper and comparison to atomistic simulations", Molex Corp., Tokyo, Japan, March 5, 2012.
5. M. A. Gosálvez, "Nucleation and growth kinetics of graphene on Cu", Aalto University, Helsinki, Finland, February 24, 2012.
6. M. A. Gosálvez, "Evolutionary atomistic methods for the simulation of surface processing with applications in microengineering", NanoGune, Donostia - San Sebastián, Spain, November 14, 2011.
7. M. A. Gosálvez, "Evolutionary atomistic methods for the simulation of surface processing with applications in microengineering", Aalto University, Helsinki, Finland, October 17, 2011.
8. M. A. Gosálvez, "Evolutionary approach for the simulation of surface processing with applications in microengineering", Tampere University of Technology, Tampere,

Finland, October 13, 2011.

9. M. A. Gosálvez, "Recent advancements in the simulation of anisotropic etching for microengineering applications", Laboratory for Micro-Nano Medical Device, Dept. of Mechanical Eng, Southeast University, Nanjing, China, June 10, 2011.
10. M. A. Gosalvez, N. Ferrando, P. Pal, Y. Xing, J. Ohara, and K.Sato, "New features in IntelliEtch", Jiangsu IntelliSense Technology Co., Ltd., Nanjing, China, February 24, 2010.
11. M. A. Gosálvez, "An overview of anisotropic etching and its simulation", Jiangsu IntelliSense Technology Co., Ltd., Nanjing, China, February 12, 2009.

H. Stays in internationally recognized centers:

Over 13.5 years abroad:

1. University of Kent at Canterbury, Canterbury, UK, 1994-1995 (9 months)
ERASMUS student, Fourth year studies in Physics with Materials Physics

2. X-ray Laboratory, University of Helsinki, Helsinki, Finland, 1996-1998 (1.5 years)
Bilateral exchange student, Structural studies using single crystal diffraction experiments

3. Physics Lab., Helsinki Univ. of Technology, Helsinki, Finland, 1998-2003 (5 years)
PhD student, Atomistic Modeling of Anisotropic Etching of Crystalline Silicon

4. Sato Lab., Dept. Micro-Nanosystems Eng., Nagoya Univ., Japan, 2004-2007 (3 years)
Postdoctoral research, Modeling of Anisotropic Etching for MEMS Applications

5. Physics Lab., Helsinki Univ. of Technology, Helsinki, Finland, 2007-2008 (2 years)
Postdoctoral research, Modeling of Anisotropic Etching for MEMS Applications

6. Sato Lab., Dept. Micro-Nanosystems Eng., Nagoya Univ., Japan, 2009-2010 (1.5 years)
Postdoctoral research, Modeling of Anisotropic Etching for MEMS Applications

I. Supervised thesis: (4)

1. Teemu Hynninen, **PhD Thesis**, "*Multiscale modeling of effects due to impurity clustering in semiconductor systems*", Helsinki University of Technology, Faculty of Information and Natural Sciences, Department of Applied Physics, Finland, 2008.
Grade: Top grade ("With distinction")

2. Néstor Ferrando, **PhD Thesis**, "*Estudio, Modelado e Implementación Paralela de Sistemas Celulares Utilizados en Microfabricación*", Universitat Politècnica de València, Departamento de Ingeniería Electrónica - Departament d'Enginyeria Electrònica, Spain, 2011.
Grade: Top grade ("Cum laude")

3. Di Cheng, **PhD Thesis**, "*Characterization and modeling of anisotropic wet etching of crystalline silicon and quartz*", Nagoya University, Dept. of Micro Nanosystems Engineering, Dept. of Mechanical Engineering, Japan, 2006.
Grade: No grading system used for PhD Thesis in Nagoya University

4. Carles Montoliu Álvaro, **M.Sc. Thesis**, "*Implementación del método Level Set para la simulación del proceso químico de atacado anisótropo húmedo aplicado para la microfabricación*", Universitat Politècnica de València, Departamento de Ingeniería Electrónica - Departament d'Enginyeria Electrònica, Spain, 2012.
Grade: Top grade ("Cum laude")

J. Other supervision:

Exchange students

1. Yan Xing (2005-2007, Nagoya University). Bilateral MEXT scholarship program between Japan and China. *Highlight of results:* simulation program VisualTAPAS, leading to a licensing agreement with IntelliSense Software Corp. (see Section *C. Technology transfer/participation in research contracts with companies*) and numerous publications (see Section *G. Publications*).

Special assignments by undergraduate students

2. Jussi Leinonen (May–Aug 2003, Laboratory of Physics, Helsinki University of Technology, Finland), *Formation of shallow round pits on anisotropically etched Si(100)*.
3. Anssi Paalanen (May–Aug 2003, Laboratory of Physics, Helsinki University of Technology, Finland), *Non-Arrhenius behaviour during anisotropic etching of crystalline silicon*.

Final year projects by undergraduate students (Proyectos de Fin de Grado/Carrera)

4. Karmele Valencia Guinot (year 2017/2018, Facultad de química, Universidad del País Vasco UPV/EHU), Implementación y validación de reacciones elementals sober superficies para el analysis de la energía de activación aparente en catálisis heterogénea.
5. Estíbaliz Sánchez Izquierdo (year 2014/2015, Facultad de informática, Universidad del País Vasco UPV/EHU), *Concepción, diseño e implementación de un software multinivel para el servicio Morfokinetics*.
6. Daniel Franco Barranco (2014/2015, Facultad de informática, Universidad del País Vasco UPV/EHU), *Paralelización mediante OpenMP de segmentación de imágenes para el análisis de materiales bidimensionales*.

K. ***Teaching***

Lecturer:

#	*Code*	*Course name*	*Hours*	*Term*
Universidad del País Vasco UPV/EHU, Facultad de Química Grado en Química				
1	26137	Matemáticas II y Estadística	60	Spring 2019
Universidad del País Vasco UPV/EHU Master in Nanoscience				
1	502798	From Nanoscience to Nanotechnology	8	Spring 2019
Universitat Politècnica de València:				
1	Interdisciplinar M.Sc. studies	Automatas Celulares y Monte Carlo cinético: Métodos atomísticos para la propagación de superficies, con aplicaciones en sistemas microelectromecanicos MEMS	8	April 2012
Nagoya University:				
2	Interdisciplinar M.Sc. studies	Theoretical-practical aspects of KMC and CA methods for interface propagation problems	10	August 2009
3	6892	Silicon Micromachining (*invited lecture*)	2	Spring 2009
4	6892	Silicon Micromachining (*invited lecture*)	2	Spring 2006
Helsinki University of Technology:				
5	Tfy-3.468	Surface Physics (*invited lecture*)	2	Autumn 2007

Teaching assistant:

#	*Code*	*Course name*	*Hours*	*Term*
University of Helsinki:				
6	553394	Physics I (Mechanics)	54	Autumn 1997
7	553395	Physics II (Electromagnetism)	28	Spring1998
8	553395	Physics III (Waves)	28	Spring1998
Helsinki University of Technology:				
9	Tfy-3.13	Physics I (Mechanics)	27	Autumn 1998
10	8		27	Autumn 1999
11			32	Autumn 2001
12			27	Spring 2002
13			27	Autumn 2002
14	Tfy-3.13	Physics II (Electromagnetism)	27	Spring 1999
15	9		27	Spring 2000
16			32	Autumn 2001
17			27	Spring 2002
18			27	Autumn 2002

19	Tfy-3.125	Physics II (Electromagnetism, in Finnish)	27	Spring 2000
20	Tfy-3.102	Physics I (Mechanics, in Finnish)	27	Autumn 2000
21 22	Tfy-3.362	Solid State Physics I	27 27	Spring 2001 Spring 2002

L. Referee for peer-reviewed journals:

Gosálvez has served as a referee/reviewer for the following peer-reviewed journals:
•Applied Physics Letters (APL by American Institute of Physics, AIP)
•Computer Physics Communications (CPC by Elsevier)
•Journal of Crystal Growth (by Elsevier)
•Journal of the Electrochemical Society (JES by the Electrochemical Society, ECS)
•Journal of Microelectromechanical Systems (JMEMS by IEEE/ASME)
•Journal of Micromechanics and Microengineering (JMM by Institute Of Physics, IOP)
•Journal of Molecular Catalysis A - Chemical (by Elsevier)
•Journal of Physics: Condensed Matter (JPCM by IOP)
•Materials Science in Semiconductor Processing (MSSP by Elsevier)
•Modelling and Simulation in Materials Science and Engineering (MSMSE by IOP)
•Nanotechnology (by Institute Of Physics, IOP)
•Sensors (by MDPI, Switzerland)
•Sensors and Actuators A: Physical (SNA by Elsevier)
•Sensors and Materials (by MYU, Tokyo, Japan)
•Simulation Modelling Practice and Theory (SIMPAT by Elsevier)
•Surface Science (by Elsevier)
•Surface and Interface Analysis (SIA by Wiley)

M. Professional skills:

Programming, knowledge transfer and teaching, research group supervision, coordination and management, capacity for abstraction and analysis, good communication and social skills, positive thinking, strong will, full exploration of possibilities for problem solving, strong endurance, analytical decision making.

N. Computers and programming:

TAPAS

TAPAS (or Three-dimensional Anisotropic Processing at All Scales) is a FORTRAN 90 program for the simulation of anisotropic etching of silicon, developed by M. A. Gosálvez during 1999 - 2006. It has been used for the completion of 14 scientific publications in international peer-reviewed journals and two PhD Thesis (M. A. Gosálvez, 1999-2003, HUT and T. Hynninen, 2006-2008, HUT)

VisualTAPAS (IntelliEtch 1.0)
IntelliEtch (also known as VisualTAPAS) is a Visual simulator of Three-dimensional Anisotropic Processing at All Scales originally developed by M. A. Gosálvez and Y. Xing during 2005-2008 (www.fyslab.hut.fi/~mag/VisualTAPAS/Home.html). VisualTAPAS is a self-contained, user-friendly, multiscale atomistic simulator of anisotropic etching with multi-masking capabilities based on an octree representation of the silicon sample. It uses both Kinetic Monte Carlo (KMC) and Cellular Automata (CA) algorithms for propagating the surface forwards in time. In addition to assisting in the engineering design of MEMS structures, VisualTAPAS enables a deeper insight of key features such as the atomistic structure of any surface orientation, the step flow nature of wet etching or the development of characteristic morphologies in the evolving multifaceted etch front. Since 2008 VisualTAPAS has been licensed to IntelliSense Software Corp., Boston, Massachusetts, US, for marketing around the world under the name of IntelliEtch (www.intellisensesoftware.com/modules/IntelliEtch.html).

IntelliEtch 2.0
IntelliEtch 2.0 is the newly developed version of the wet etching simulator licensed in 2010 to IntelliSense Software Corp., Boston, Massachusetts, US, for marketing around the world (www.intellisensesoftware.com/modules/IntelliEtch.html). The software has been developed by M. A. Gosálvez, N. Ferrando and Y. Xing during 2009-2010. Thanks to the combined efforts by M.A. Gosalvez, P. Pal and K. Sato, IntelliEtch 2.0 contains the largest wet etching database ever developed for wet etching simulations with more than 30 etchants. IntelliEtch 2.0 incorporates a recent, major advancement in the simulation of wet etching using the CCA method, namely, a novel, fast, parallel implementation of the CCA method based on performing most calculations by using the large computing power of recently available, inexpensive graphics cards (GPUs). Our GPU implementation of the CCA method achieves simulation speeds that are typically two orders of magnitude faster over a traditional computation on a single Central Processing Unit (CPU).

IntelliEtch 2.0 consists of four applications: (1) IntelliEtchC (IEC), the CPU-based engine of the wet etching simulator based on Kinetic Monte Carlo (KMC) and Cellular Automata (CA) methods in different flavors, such as Basic CA (BCA), Simple CA (SCA) and Continuous CA (CCA). (2) IntelliEtchG (IEG), the GPU-accelerated version of the wet etching simulator based on the Continuous CA (CCA) method. (3) Wagon Wheel Analyzer (WWA), a tool to extract experimental etch rates from optical images of <110>- and <100>-oriented DRIE micromachined silicon wagon wheels that are subsequently wet etched in anisotropic etchants; and (4) Etch Rate Visualizer / CCA calibrator (ERV), a tool to visualize the complete orientation dependence of the etch rate for all possible crystallographic orientations in the unit sphere based on one of two possible inputs: (i) the experimental etch rates obtained using the Wagon Wheel Analyzer, or (ii) the initial and final positions of the silicon surface for simulation/experimental wet etched silicon hemispheres.

Based on the visualized etch rates for a given etchant, the tool can be used to calibrate the CCA method and thus perform wet etching simulations for that etchant using both IEC and IEG.

IntelliEtch 2.21
IntelliEtch 2.21 is the newest version of the wet etching simulator (see IntelliEtch 2.0 above). In addition to the previous features, this version enables the simulation of (1) anisotropic etching of quartz, and (2) wet/spray etching of metals (non-trivial quasi-isotropic etching).

Role as developer of VisualTAPAS / IntelliEtch:
(i) Knowledge transfer - to initially provide guidance and explicit directions about the algorithms, procedures, methods and data structures, based on previous programming experience in the writing of TAPAS as well as in the development of KMC and CA simulations. (ii) Algorithm development - to explore new implementations, leading to the analytical solution of the discrete and continuous CA methods as well as more efficient implementations of the continuous CA method. (iii) GUI design - to ensure a functional, yet simplified design for the Graphical User Interface of the tool. (iv) Web page design, realization and maintenance. (v) Testing and debugging the tool. (vi) Documentation - user manuals and numerous tutorials, presentations and movies. (vii) Management of intellectual property rights and licensing agreements. (viii) Business and marketing - development of business plan and expansion scheme for the tool, including meetings with investors and negotiations.

Operating Systems (best to worst knowledge): Mac OS X, UNIX/Linux, Windows.

Programming (best to worst knowledge)
Fortran 90 and 77, basics of C++, basics of MPI. Fair experience with debuggers.

Numerical analysis, data processing and visualization
Advanced use of scripts and functions in MATLAB (and clones such as Scilab).
Experience with GNUPLOT, C-PLOT, SPEC, MATHEMATICA, and others.
Wide experience in the visualization of point clouds *e.g.* as surfaces
(Delaunay triangulations, Voronoi diagrams, lighting, ...)